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EUROPEAN REACTING FLOW RESEARCH: A FINAL ASSESSMENT(U)
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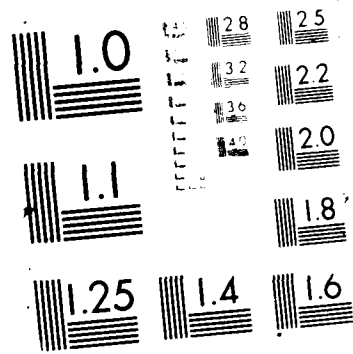
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European Reacting Flow Research: A Final
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Eugene F. Brown

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19 ABSTRACT (Continue on reverse if necessary and identify by block number) The author provides a sampling of combustion research activities in Europe, with emphasis on the work in France, West Germany, and the UK. He states that there is a great deal of diversity in the projects, and in most cases there is strong industrial support. He also reports on the important new European initiatives--the European Communities Combustion Research Program and the European Center on Flow, Turbulence, and Combustion Simulation.			
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EUROPEAN REACTING FLOW RESEARCH: A FINAL ASSESSMENT

1 INTRODUCTION

During the period from 1 September 1985 to 31 August 1987, I was the Liaison Scientist for Fluid Mechanics at the London Branch Office of the Office of Naval Research. My research interests are in the area of computational fluid dynamics (CFD) and although my visits and conference attendance were rather broad in coverage, much of what I have written in the form of ESN articles and ONRL reports tended to concentrate on the computational fluid dynamics. In this final assessment report I would like to review European research activities in reactive flows--that is, flows in which combustion is present--from the same perspective.

My decision to assess reacting flow research was motivated on the one hand by a strong ONR interest in the problems of reacting flows (witness the recent Accelerated Research Initiatives in combustion instabilities and supersonic combustion) and on the other by the fact that reactive flows are perhaps the supreme test of modern computational techniques because reactive flows have short temporal scales which render the model equations stiff and therefore resistant to solution and small spatial scales which place severe constraints on the spatial resolution of the calculations. In what follows, I will be reporting on international European programs in combustion and then on European research in combustion on a country by country basis. In addition, I will be reporting on developments in computational fluid dynamics which, although not at present being used in a combustion context, appear to me to have relevance to the solution of combustion problems.

2 INTERNATIONAL EUROPEAN ACTIVITIES

European Research Center on Flow, Turbulence and Combustion Simulation

Prospects are good that a European center for the numerical simulation of combustion, fluid mechanics, and turbu-

lence problems will be established. The intention of the European Research Center on Flow, Turbulence and Combustion Simulation is to mobilize the research sectors of the European countries in defense of what is perceived to be the economic threat of high-technology, computer-designed industrial and domestic products from the US and Japan. A formal proposal was drawn up approximately 2 years ago and at least four meetings have been held to discuss strategies for the center's organization, function, and support. The center would consist of a collection of, say, five interconnected supercomputers of the Cray X-MP class and a visiting and resident staff of scientists and engineers working in a structure somewhat along the lines of the Institute for Computer Applications in Science and Engineering (ICASE) at the NASA Langley Research Center in the US. The facility would be networked to satellite centers in each European country. Professor Charles Hirsch of the Free University of Brussels (Belgium) is chairman of the organizing committee.

Several European countries have volunteered to provide the facilities to house the center, and financial support from a number of European industries has been pledged. It appears that funding from the European Economic Community will not be forthcoming and, therefore, the success of the venture depends upon the ability of each of the national delegates to secure funding from his own country. This will not be an easy task for a variety of reasons. First of all, not all of the European high-technology (aerospace and automobile, for example) manufacturers are convinced of the utility of such a center. Second, there are competing (or apparently competing) European organizations such as the French European Center for Research and Advanced Training in Scientific Computation (CERFACS) which may give certain European nations (especially France) second thoughts about establishing another center. Finally, instead of the proposed center some delegates appear to prefer a loose affiliation of already existing European laboratories and research organizations. The



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unique feature of the proposal as I see it, in comparison with the NSF-sponsored centers for computational excellence in the US, is its industrial orientation. If the center becomes a reality and operates as expected it will have a major influence on the products of Europe's high-technology industries.

European Communities' Combustion Research Program

A second cooperative European combustion activity is the recent initiation of a European combustion research program by the European Economic Communities (EEC). The 4-year program, which began in 1985, involves industrial, government, and industrial partners and consists of 14 complementary programs. The EEC contribution is approximately \$8 million plus an equal amount contributed by various European industries and the Joint Research Committee, which consists of six leading European car manufacturers (British Leyland, FIAT, Peugeot, Renault, Volkswagen, and Volvo). The intent of the program is to:

- o Support research on the more basic aspects of turbulent combustion including modeling, chemical kinetics, mechanisms of elementary processes, and advanced diagnostics
- o Pursue the development of global combustion models in reciprocating (Diesel and Otto cycle) engines for design optimization
- o Explore the possibilities for increasing the efficiency of Otto cycle engines and for developing high-efficiency, low-emission Diesel engines
- o Study the combustion of low-grade fuels and their effect on marine engine operation.

The program is structured to address several shortcomings of European combustion research revealed in a study by the UK Atomic Energy Research Establishment-Harwell (UKAERE-Harwell) which faulted the level of funding for combustion research in Europe, pointed to fragmented and poorly coordinated programs, and

cited difficulties in making the industrial community aware of the results of potentially interesting research. Although it is perhaps premature to assess the success of the program, the results to date are sufficiently encouraging that the Council of the European Communities is in the process of planning a 4-year follow-up program.

3 ACTIVITIES IN INDIVIDUAL COUNTRIES

France

Of all of the countries of western Europe, France appears to have the largest and most comprehensive program of combustion research. At the University of Rouen, both diffusion and premixed flames are being investigated in both experimental and numerical studies in the Laboratory of Thermodynamics. At present the laboratory is staffed by approximately 80 people. Approximately 50 percent of its research is supported by French government organizations and 50 percent by French industries. A full complement of diagnostic tools was in evidence including equipment for making OH fluorescence and Rayleigh scattering measurements for heat release and temperature measurements, and laser Doppler anemometry and laser tomography equipment for velocity measurements and flow visualization. In addition, in the internal combustion engine experiments directed by M.J. Cottureau, a special reference-beam coherent anti-Stokes Raman spectroscopy (CARS) system was in use. In the flame experiments the flame structure and topology of the flame front were of interest. In the diffusion flame experiments and in the premixed flame experiments various levels of turbulence were created by an upstream-mounted grid resulting in regions where the flame was completely extinguished. The effects of pressure gradient on the turbulence velocity and Reynolds stress was also investigated. (D. Escudie, a former student at the University of Rouen, has undertaken a similar investigation at the Laboratory of Fluid Mechanics at the Ecole Centrale de Lyon involving the study of the interaction of a single vortex street with

a wire-stabilized premixed hydrogen flame.)

R. Borghi, who is in charge of the numerical modeling work has developed the highly regarded interchange with the mean (IEM) technique by which mean reaction rates can be computed from the solution of Lagrangian equations for the concentration and temperature fluctuations. Perhaps his most novel contribution is the development of a lattice gas simulation of turbulent reacting flows. By considering separate steps in which the turbulence was simulated by a random-walk process, followed by a particle interaction step, and finally by a flame propagation step, Borghi was able to compute a mean reaction rate and to examine the influence of various time scales on the combustion process. Although such relationships are of great interest, everything hinges on the appropriateness of the lattice gas model to simulate the combustion process, and much needs to be done in this area.

At the Ecole Centrale de Paris, Professor S. Candel heads the Combustion Department of the (Centre National de la Recherche Scientifique [CNRS]) which is part of the Laboratory of Molecular Energetics and Macroscopic Combustion. The laboratory consists of approximately 55 engineers, professors, technicians, and graduate students. As at the University of Rouen, the laboratory enjoys a good relationship with French industries, primarily because of the close industrial connection of most of its combustion-related research. Candel is a young and extremely capable researcher. His most recent computational work involves the simulation of vortex combustion and employs the coherent flame model developed by Marble at the California Institute of Technology, where Candel received his Ph.D. Interesting experiments are being conducted in both self-initiated and externally-excited combustion instability in which the interaction between acoustics and combustion, including the anatomy of the feedback mechanism, is of interest. By means of simultaneous phase-averaged and spectral-imaging techniques, he compared simultaneous schlieren and

C_2 emission measurements to study the behavior of the instability process. He discovered that vortices shed from the flame holders at the combustor inlet provoke intense combustion as they proceed downstream. The intense combustion, in turn, provides the pressure pulse whose upstream propagation provokes the vortex shedding, thus sustaining the instability.

Combustion research activities directed by Professor P. Clavin have existed at the Université de Provence (Marseille) for many years and have recently been combined into the Laboratory for Combustion Research. The laboratory consists of 30 Ph.D. candidates, technicians, engineers, and staff members, and, like Candel's department in Paris, is a CNRS-supported organization. Unlike Candel's laboratory, however, Clavin has few industrial contracts and prefers to work on fundamental rather than industrially related problems. Although his group is small there appeared to be a synergistic combination of analytical, numerical, and experimental activity underway.

The experimental interests of Clavin's laboratory are in flame-front dynamics, premixed stabilized flames, flame propagation in random media, and laser diagnostics. Perhaps the laboratory's best-known accomplishment in this latter connection is the invention and refinement of the technique of laser tomography by Professor L. Boyer. On the numerical side, Clavin has been involved in the development of spectral methods, adaptive gridding, and most recently the use of cellular automata (lattice gas) for the simulation of reacting flows. In the lattice gas simulation of combustion the particle labels are allowed to change as they move about the grid in accordance with modified collision laws which permit (at least) for different kinetic energies of the burned and unburned particles. The simulations of premixed planar flames exhibited the well-known cellular structure, and the characteristic size of the cells was observed to be of the same order of magnitude as the marginally stable wavelength predicted by theoretical analysis. One must be careful in interpreting

these results since the Mach number of the flame modeled by the lattice gas method is relatively large and the coupling with acoustic modes is strong in comparison with real flames. Nevertheless, for low Mach number, low Reynolds number flows, lattice gas calculations are computationally competitive with solutions of the Navier-Stokes equations, and their simplicity and massively parallel logic make them ideally suited to special purpose, high-speed, parallel computers (of the "hypercube" variety).

At the Ecole Nationale Supérieure de Mécanique et d'Aérotechnique in Poitiers, B. Deshaies has performed an interesting experiment to verify the effects of stretch and curvature on premixed laminar flames predicted by the theory of Clavin and Joulin. A vertically-oriented "flat flame" burner was used which could be modified to produce various flame shapes ranging from a classical flat flame to an inverted curved flame. It was concluded that these experiments, in which the velocity gradient and flame front curvature were measured with LDA and laser tomography, verified the theory to within a few percent. Further experiments are underway in which seeding by submicron-sized solid refractory particles will be used to obtain an improved measurement of the velocity gradient at the flame front in order to produce an improved verification of the theory.

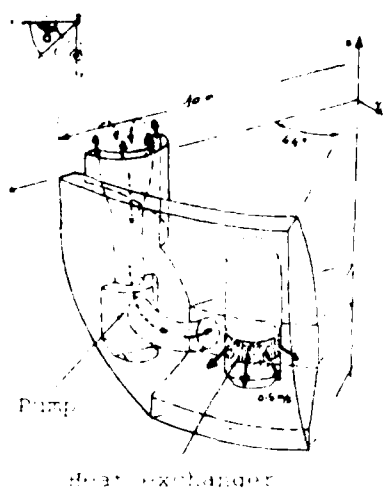
At the Sophia-Antipolis Center of the Institut National de la Recherche en Informatique et en Automatique (INRIA), B. Larrouturou has developed a finite-element flame-front calculation which automatically adjusts its fineness to accommodate the rapid variations of flow properties which are found there. The flame front is centered in the computational zone by moving the mesh forward at the local flame speed, and the proper concentration of cell size is achieved through a combination of dynamic and static rezoning using a mesh function which reflects the local "goodness" of the mesh in terms of both the truncation error and the local mesh regularity. The calculations have been applied to one-dimensional, steady, planar flame propa-

gation and two-dimensional curved flame calculations. In flame front calculations, the very strong nonlinear dependence of the reaction rates on temperature, the inherent nonlinearities in the problem, and the widely disparate time and spatial scales lead to the most efficient grid being a highly nonuniform one. For this reason, a finite element approach (such as used by Larrouturou) is ideal because of its demonstrated robustness on irregular meshes.

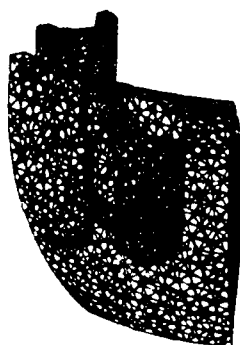
As a final example of the performance of a finite element calculation on a highly nonuniform mesh, I would like to present a nonreacting calculation done by P. Lasbleiz of the National Hydraulic Laboratory of Electricité de France (Chatou). The grid (see Figure 1) is set up to do a laminar, incompressible calculation of the flow in the cold plenum of the Super Phénix nuclear reactor. Here, of course, the spatial nonuniformity results from the very complicated nature of the flow geometry. In fact, I think this is the most complicated geometry I have ever seen attempted! It illustrates to me very clearly the effectiveness of finite element methods when dealing with problems which demand the use of meshes of highly nonuniform shape either because of geometric characteristics (as in this problem) or because of nearly discontinuous behavior brought about by internal effects (such as combustion).

West Germany

West Germany's strength seems to lie in reaction kinetics where substantial efforts are underway at the University of Göttingen and the Max-Planck-Institut für Strömungsforchung (Göttingen). Having a closer relationship with fluid mechanics, however, are the numerical studies of flame structure which are being carried out at the University of Heidelberg and the Rheinisch Westfälischen Technischen Hochschule Aachen (RWTH-Aachen). At the University of Heidelberg, B. Rogg has carried out a numerical simulation of confined methane-air diffusion flames including nonequilibrium effects. The simulation was carried out with a primitive variable modification of Smook's



(a) General view



(b) Finite element mesh

Figure 1. Super Phénix cold plenum (Lasbleiz).

(Yale University, New Haven, Connecticut) implicit adaptive-grid technique. He also examined the effect of using a simplified reaction model. In comparing the results of a 25 reaction model with a reduced mechanism consisting of four global reactions, good agreement was obtained with the available experimental data. When only a single one-step overall reaction model was used however, discrepancies arose which indicated that the accurate numerical prediction of confined laminar diffusion flames requires the use of a somewhat more complete reaction mechanism.

At RWTH-Aachen, N. Peters also looked at simplified reaction models and has developed a systematic strategy to produce reduced reaction schemes for methane, methanol, and propane. What he sought was the smallest number of steps which is algebraically tractable and yet still provides realistic flame structure. Beginning with 30 reactions for methane, 20 for methanol, and 39 for propane, Peters obtained a reduced reaction scheme consisting of four reactions for methane, four for methanol, and two for propane. These reduced schemes represent enormous computational savings when these relationships are used to examine flame structure. Peters has carried out such calculations for methane and identified a four-zone flame front (see Figure 2) including preheat zone, a fuel consumption layer, a H_2 -CO oxidation layer, and a H_2 -CO non-equilibrium layer. Peters was able to obtain an estimate the thickness of the various layers and the effect of pressure variations on the thickness of the flame front.

A CFD technique which has significant potential for combustion problems is the so-called zonal or domain decomposition approach. A particularly good example of this is the viscous transonic airfoil calculation carried out by M. Schmatz of Messerschmitt-Bölkow-Blohm GmbH (Munich). As the words imply, domain decomposition means subdividing the original computational domain into a number of subdomains. This has a number of

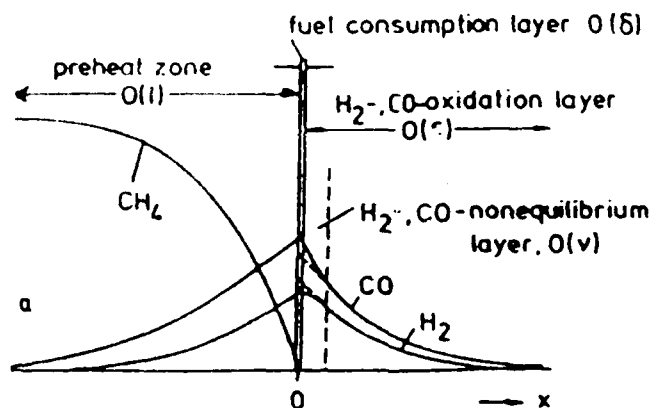


Figure 2. Inner structure of premixed Methane-air flame (Peters).

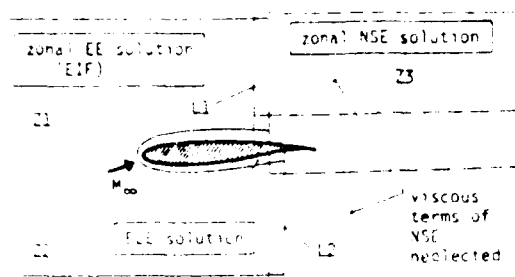


Figure 3. Domain decomposition applied to an airfoil calculation: EE = Euler equations, NSE = Navier-Stokes equations, BLE = boundary layer equations (Schatz).

important advantages. In Schatz's case it allowed him to use a simpler set of model equations (the Euler equations) in regions away from the walls and upstream of shocks where viscous effects were expected to be small. Figure 3 provides an indication of how the calculation was carried out. In combustion problems, the zonal approach could be used to separate the regions where equilibrium chemistry could be used from regions where reaction kinetics is needed. Another possibility would be to divide the reacting flow into regions according to expected temporal and spatial scales so that in each region optimal algorithms and discretization schemes could be used.

United Kingdom

Internal combustion engines are the focus of much of the combustion research activities in the UK. For example, at KAERE-Harwell, C.R. Negus is studying the structure of high-pressure (Diesel) sprays under both nonreacting and reacting conditions. Similar studies are being done by A. Yule at the University of Manchester Institute of Science and Technology (UMIST) and by A. A. Hamidi of the University of Sheffield.

The Center for Combustion and Energy Studies at the University of Leeds is an interdisciplinary laboratory consisting of 13 permanent staff members and 15 research students; it was founded in 1967 by Professor P. Gray of the Department of Physical Chemistry, Professor G. Dixon-

Lewis of the Department of Fuel and Energy, and Professor D. Bradley of the Mechanical Engineering Department. The combustor modeling activity is directed by Dr. P. Gaskell and involves both experimental tests and development of numerical models for jet-stirred, dump, and gas turbine combustors. In preliminary numerical modeling of jet-stirred reactors, Gaskell discovered that with the Pandakar and Spalding scheme the numerical viscosity present in the original hybrid algorithm completely swamped the improvements which should result if more sophisticated turbulence models are used. This led Gaskell to adopt the quadratic up-wind interpolation (QUICK) scheme. However, in a related but nonreacting calculation, Gaskell discovered that the QUICK scheme runs into difficulty in regions of high shear because of the unbounded characteristics of the algorithm. Recently he has developed what he calls his curvature compensated convective transport (CCCT) scheme, which fulfills the necessary requirement for boundedness. This is similar in spirit to the monotonicity-preserving scheme introduced by Boris (NRL) in his flux-corrected transport (FCT) scheme.

In turbulent explosion experiments, directed by Mr. M. Lawes, the effect of high turbulence levels on burning rate is being examined. In these tests a region of isotropic turbulence is produced and then ignited by a single or dual-spark arrangement, producing a spherical flame. Turbulence intensities of sufficient magnitude can be achieved to produce flame extinction. Gas turbine combustor experiments are being done by Dr. C. Shepard using conventional five-hole probes and crossed hot-wire probes. He found that the inlet velocity profile of the dilution jets was extremely nonuniform and that computational codes developed to predict gas turbine combustor flows must include this nonuniformity if accurate results are to be expected. Finally, in the internal combustion engine research--supported by British Leyland and also directed by Shepard--single-cylinder, two-spark-head internal combustion engines are being used to study

the effect of torch-ignition on combustion enhancement in various types of pre-combustor geometries.

Gas turbine combustors are also an important research topic in the mechanical engineering department at Imperial College (London). Here, in the Fluid Mechanics Section, headed by Professor J. Whitelaw, experiments have been undertaken for a number of years to obtain a better understanding of the combustion process and to obtain data for the construction of improved numerical models being developed at Imperial College under Rolls-Royce sponsorship by W. P. Jones of the Chemical Engineering Department. Whitelaw has been involved in experiments on turbulent premixed combustion for many years. He has performed experiments on disk-stabilized flames in which he has made detailed measurements of the velocity, temperature, and concentration fields by using laser velocimetry, small-diameter thermocouples, and gas sampling probes. His experiments revealed that nongradient diffusion plays an important role in gas turbine combustor flows. He also looked at a series of experiments with bluff-body-stabilized premixed flames in ducts and examined the acoustic character of the oscillations. This work is being done under ONR contract and is directed toward obtaining an improved understanding of combustion instabilities in ramjets.

Other European Countries

In Italy, internal combustion engine research is being carried out at the Centro Nazionale di Ricerca sulla Tecnologia della Propulsione e la Materiali (CNPM) in Milan, and research on engine combustion, fluidized bed combustion, and spray characteristics is being done at the Istituto di Ricerche sulla Combustione in Naples. My impression is that the experiments (particularly the engine combustion experiments) are rather conventional in character and specific to the engine being tested. Consequently, the data is primarily of design rather than research interest. In addition, the internal combustion engine modeling which I

saw tended to be rather conventional and uninspired.

In Spain, there are only two universities where combustion research is being conducted: the Politechnic University of Madrid and the University of Zaragoza. Their efforts are small in terms of the number of people involved but represent high-quality activities. At the Politechnic University of Madrid, the combustion research is being done by Professor A. Liñan, whose current research interests include theoretical studies of the effect of simplified reaction models on flame properties, the structure of diffusion flames, and numerical models for the description of flame propagation in laminar mixing layers. At the University of Zaragoza Professor C. Dopazo's interests are in both the theoretical and experimental aspects of turbulent combustion. He is internationally recognized for his work on Monte Carlo simulation of turbulent reacting flows. His current research involves carrying out experiments and developing computational models for heavy-oil-fueled industrial burners for a Spanish electric-power generating utility. His laboratory seems to be reasonably well equipped: however, there is a shortage of well-trained scientific personnel to carry out the experiments.

Table 1 provides an interesting comparison of the European contributions to combustion research with those of the US in terms of the number of papers presented at the 21st International Symposium on Combustion, which was held in August of 1986 in Munich. This conference is run every 2 years and is organized by the Combustion Institute, which has chapters in each of the European countries and most of the industrialized nations throughout the world. Of the Western European nations, France, the UK, and West Germany are by far the largest contributors, with Italy and Spain trailing far behind.

4 CONCLUSIONS

I have attempted to provide a sample of combustion research activities in

TABLE 1
U.S. and European Contributions to the
21st International Symposium on Combustion
Munich, West Germany (3-8 Mar 1986)

Subject	US	EUROPE					
		France	UK	West Germany	Italy	Spain	Other
Coal combustion			5		2	1	
Spray combustion	8				1		
Combustion diagnostics	7			2			
Turbulent combustion	22	3	3	3			1
Ignition/extension	2		2	1			2
Reaction kinetics	16	1	2	7			3
Solid repellants	5						
Laminar flames	8	1					
Detonation & explosion	4		2				2
Combustion-generated pollutants	13	3	1	4	1		
Practical combustion systems	6	1	3				2
Fire	9			2			
Total	100	8	19	19	4	1	11

Europe with emphasis on France, West Germany, and the UK where most of the research seems to be taking place. There is a great diversity in the projects which are being undertaken and in most cases a strong industrial interest in the more applied areas as evidenced by significant financial support especially in France and the UK. Good contact with the US combustion research community was evident, particularly in France and the UK, with frequent international exchanges being the rule rather than the exception. Within Europe what had at one point been identified as a problem in terms of co-ordination and communication among scientific and the industrial sectors appears to have been affectively addressed with the new European Communities Combustion Research Program. This program and the proposed European Center on Flow, Turbulence, and Combustion Simulation are important new initiatives and should be closely watched by US investigators for

the opportunities which they may provide for further strengthening US/European collaborative research on this topic.

APPENDIX A

Addresses of investigators mentioned in this report.

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APPENDIX B

European Science Notes (ESN) articles which I have written which contain additional information about the activities described in this report are:

- 40-3:111* European Computing Center for Turbulence and Combustion
- 40-4:133 Fluid Mechanics, Combustion, and Hydroacoustics at Bertin

40-4:136 Fluid Mechanics Research at Laboratoire National d'Hydraulique
40-4:143 EUROMECH 203, Combustion Theory

1987

41-1:51 French Supersonic Combustion Research--Revisited
41-3:156 Combustion Research at Ecole Centrale Paris
41-4:213 Combustion Studies at the Laboratory of Thermodynamics,
The University of Rouen
41-5:256 First International Symposium on Domain Decomposition Methods
41-5:273 Combustion and Energy Studies at the University of Leeds
41-5:275 Research and Development Activities in Fluid Mechanics at
Rolls-Royce
41-6:332 Harwell Laboratory Participating in European Combustion Initiative
41-8:437 EUROMECH 220: Mixing and Chemical Reactions in Turbulent Flows
41-9:508 Fluid Mechanics Section, Imperial College, London

(To appear) Fluid Mechanics and Combustion Research in Spain
(To appear) Workshop on Mathematical Modeling in Combustion
(To appear) Joint Meeting of the US and Italian Combustion Societies
(To appear) Joint US-France Workshop on Turbulent Reactive Flows

*Article contained in ETW, Volume 40, Issue 3, beginning on page 111.